BUILDING ISLANDS IN THE SWAMP: DIRECTIONS FOR BASIC RESEARCH IN MECHANICAL BEHAVIOR

J.W. Morris, Jr.
Department of Materials Science, University of California, Berkeley and
Center for Advanced Materials, Lawrence Berkeley National Laboratory

This paper focuses on future directions for research in mechanical behavior, with emphasis on the methodology of that research. The development of a quantitative theory of mechanical behavior is a very difficult problem, essentially because mechanical behavior is sensitive to microstructure, and microstructure can only be described precisely in a few ideal cases. Most of the interesting problems in mechanics of materials are unsolvable, and will remain so, even given the development of larger computing machines. To make progress in this area, materials scientists need to be selective and clever. There is a set of limiting problems that can be solved exactly. These should be solved and their consequences exploited. The bulk of the field is filled with problems that cannot be solved exactly, but can often be mastered by approximate techniques that are adequate to predict and control mechanical properties to the level required for modern technology. The exploitation of these approximate methods is, in fact, the way materials scientists have worked to achieve the substantial progress we have made in recent years. To maximize future progress, it is important to recognize that we act in this way, not because our field is primitive or unscientific, but because this is the natural and appropriate way to drain the swamp in which we live.

Although much of what I am going to say in this paper pertains to materials science as a whole, I will focus my remarks on the problem of mastering the mechanical behavior of materials. I do this both because I am a bit more familiar with the mechanical properties of materials than with the chemical or electromagnetic properties, and because mechanical behavior confronts the reality of microstructure more immediately and directly than any other behavioral mode.

MECHANICAL BEHAVIOR SETS HARD PROBLEMS

While we materials scientists are, collectively, entitled to brag about the very real progress we have made, there are large gaps in our understanding of mechanical behavior. At the risk of restating the obvious, let me begin with a comment or two on why the problem is difficult. It is important to keep this in mind. We would not need so many clever and devious models if it were possible to master mechanical behavior with a frontal attack.

The problem is difficult because we can't count high enough to do a clean theory, and can't see clearly enough to do a clean experiment.

The counting problem is inherent, and comes from the nature of materials science itself. The properties of a material are determined by its composition and its microstructure. The composition is the atoms that are present. The microstructure is how they are arranged. Since there are roughly 10^{22} atoms in a cm^3 of solid, enumerating how they are arranged is an impossible task unless some simple rule does the job for us.

There are three (and, I believe, only three) cases in which the microstructure can be precisely quantified: the perfect crystal, whose periodicity locates the positions of the atoms, the perfect glass, whose randomness locates the atoms in a statistical sense, and the equilibrium state, whose microstructure may be unknown, but is, nonetheless, uniquely specified by the values of the thermodynamic coordinates. These are the microstructures that physicists study. Materials scientists must also deal with the rest. Most of the time, it is "the rest" that is important. There are no perfect crystals or perfect glasses in nature, and most of the materials that matter have been carefully manipulated out of equilibrium to achieve microstructures with useful properties.

Given that computers become bigger and more powerful every year, can we just overwhelm the complexity of microstructure? Unless we find some radically new approach, we cannot. Since groups of dislocations have an effective interaction range of 10 μm or more and evolve on a time scale of at least seconds, an *ab initio* calculation of the deformation of a dislocated metal would require treating clusters of roughly 10^{16} atoms for more than 10^{15} time steps. The best available *ab initio* codes on the biggest available machines can handle about 200 atoms, in a quasistatic configuration, so we are many, many orders of magnitude short of what is needed. But there are still more fundamental issues. Even if we could handle 10^{16} atoms, how would we know if the configuration that was modeled reproduced the salient microstructural features of the material we were trying to understand?

The experimental problem is equally difficult. Only very thin foils are transparent to the high-resolution microscopes that can follow the local behavior of dislocations. But the mechanical behavior of thin foils is not ordinarily representative of the bulk. It follows that mechanistic analyses must usually be done on samples that are cut from deformed bulk specimens. But these are frozen in space and time. It is never obvious how the dislocation network found in the foil was actually evolving at the time the test was stopped. Given the heterogeneity of plastic deformation, it is rarely even clear that the particular slice of material that appears in the sample was actually participating in the deformation at the time the test was stopped. We have learned, and are learning a great deal of value from high-resolution studies of dislocation behavior, but there are very definite limits to how far these studies can take us by themselves.

So the problem of mechanical behavior is very difficult. But it is not completely intractable, as shown by the very significant progress we have made over the years in understanding, controlling and improving mechanical properties. The gap that separates us from our objective is not so much a chasm as a swamp; a land that can be traversed, but only with great difficulty, and then only by studiously avoiding the quicksands and impenetrable thickets that cover so much of its interior.

How do we best proceed? In the time-honored method for bringing swampland into productive use, one begins by securing the high ground, the dry islands that are occasionally found in any swamp. One expands these by draining along the periphery, and makes new islands in the spaces between by locating other places where the swamp is shallow and easily drained. The latter effort requires tools for prospecting and draining that may be very different from those that are used to develop property on dry land. Eventually, one hopes to create a population of dry places that can be joined with bridges, making high roads that cover the swamp and percolate through it to the far side.

A parallel (and, for some, more intellectually appealing) example can be found in the development of theoretical physics prior to the advent of big computing machines. Partial differential equations that cannot be solved can, nonetheless, often be mastered by a piecewise analysis. The theorist uses a variety of techniques to obtain exact solutions at special points, uses perturbation methods to cover the immediate neighborhoods of these, and develops series expansions to bridge the gaps between them.

It is both possible and sensible to approach the problem of mechanical behavior in a similar way. Given recent advances in theoretical techniques and computational machines, there are a number of important, well-posed problems that can now be solved exactly (there are islands in this swamp). These address elastic behavior and the limits of strength, and form a solid basis for understanding and predicting a variety of mechanical mechanisms and mechanical properties. We should solve them, and thoroughly explore their implications. To make further theoretical progress, we are forced to rely on approximate models. The challenge is to construct models that help us reach the several different goals we have in studying mechanical behavior: understanding fundamental mechanisms, predicting mechanical properties, and developing superior materials. (That is, to create new islands of understanding.) To do this, it is important to recognize and exploit the full range of analytic tools that are available to us. These include a variety of different approaches to mathematical modeling, and also include qualitative and semi-quantitative methods which, in fact, often produce the most important insights.

SOLVING THE PROBLEMS THAT CAN BE SOLVED

Some problems can be solved exactly, beginning from fundamental theories at the atomic level. While I cannot claim to offer a comprehensive list, for the last three years we have had a small working group at Berkeley that has maintained a joint research program and held a biweekly seminar on this subject. We have concluded (as have a number of people in other laboratories) that there are three important problems in the mechanical behavior of ordered crystals that can now be solved *ab initio*: elastic deformation, specifically including the elastic moduli, the theoretical shear and tensile strengths that define the upper limit of strength, and the effective Peierls-Nabarro stress that defines the lower limit of strength in ductile materials at normal temperature.

It is now possible to calculate elastic moduli to an accuracy that approaches the best that can be done experimentally [1]. We have, in fact, used this capability to resolve dis-

crepancies in the published values of elastic constants. The value of this exercise goes beyond the ability to predict elastic behavior. The elastic modulus is also the first-order determinant of plasticity and fracture. For materials with given bond type, mechanical hardness scales linearly with the shear modulus (albeit with a significant scatter) [2]. The Peierls-Nabarro stress of materials with given crystal structure is largely determined by the shear modulus [3], as is the efficiency of hardening by microstructural obstacles [4]. Both classic models [5] and *ab initio* calculations [6,7] suggest that the elastic instabilities that determine the upper limits of strength also scale with the elastic modulus. A clear understanding of differences in modulus will clarify the fundamental reasons that materials have different strengths and may suggest new ways of controlling them [8].

It is also possible to calculate upper bounds for strength in shear or tension. The maximum stress a material can possibly sustain is that which destabilizes the lattice itself; at this point, the elastic limit, it must deform [9]. Over the past few years, several workers have solved this problem for various constrained deformation modes [6,10-13]. It can now be solved for unconstrained shear [7]. The solutions have several interesting features. First, they set upper limits on strength that can be used to judge possibilities (e.g., is it worth trying to harden diamond? The answer is almost certainly "no" [14].). Second, they clarify the mechanisms of instability. For example, even though Al has a high stacking fault energy, it is weakest when sheared in <11$\bar{2}$> on (111). Third, they reveal large-strain behavior that is difficult to access experimentally. For example, Al and Cu have very different relaxation patterns in finite shear on {111} [15].

We believe that it is also possible to calculate the effective Peierls-Nabarro stress, defined as the minimum stress necessary to move a dislocation. This stress sets the lower bound on the strengths of ductile materials. The calculation is made difficult by the fact that the best *ab initio* codes can handle only a few hundred atoms, so an exact calculation requires that one find a way to treat the dislocation with periodic cells of this size. Various approaches are described by Bulatov, et al. [16]. Chrzan and co-workers [17] have recently found how to construct periodic cells that appear to produce reliable results.

The outstanding methodological problem in calculating the limits of strength is to include thermal effects. While the (admittedly limited) data suggests that the elastic limit does not have a strong temperature dependence, the effective Peierls stress does, with the consequence that materials like Si and TiC, which do not exhibit dislocation plasticity at low temperature, become ductile when the temperature is sufficiently high.

A problem common to all the *ab initio* methods is that the calculations are time-consuming. Even assuming strong support, it will take years of effort to calculate and understand the limits of strength for a representative sampling of the important materials. On the other hand, if these calculations are done correctly, they will not need to be redone. For the first time, we are in a position to complete and "bank" solved problems in the mechanical behavior of real materials.

SOLVING THE PROBLEMS THAT CANNOT BE SOLVED

The mechanical behavior of materials with real microstructures can only be treated approximately. While this fact may be unsatisfying intellectually (and an embarrassingly large fraction of investigators pretend it isn't true), it does not usually present an insurmountable technological barrier. The level of accuracy that is actually required to handle the critical materials problems in modern technology is usually not all that high. Theories of mechanical behavior are used to understand materials, to predict their properties and to improve their properties. The most blatantly quantitative of these activities is prediction, and even there we are often satisfied with rather crude approximations. It is often sufficient to predict that a particularly material will have properties that are comparable to, or properties that are better than those of some other material that is known to be acceptable, without worrying too much about precisely what those properties are.

In fact, in the science of mechanical behavior the qualitative to semi-quantitative models that illuminate mechanisms are often much more useful than the quantitative theories that produce numbers. The reason is, again, inherent to materials science. The microstructural complexity that makes it so difficult to calculate mechanical behavior also makes it difficult to create materials that behave in a strictly predictable way. For example, the ultimate tensile strengths of typical structural alloys have a log-normal distribution with a standard deviation of 10% or more [18]. Even rather crude models can often "guess" the UTS to within this level of accuracy, so it is unclear what one would do with an accurate, first-principles model. If we made the enormous computational effort that would be required to compute the UTS of an engineering alloy to within a fraction of a percent, how would we know if we were right? And what would being "right" mean when the property itself has a broad natural scatter? The metallurgical community is ordinarily much more interested in mechanistic models that suggest how to narrow the scatter, or how to extrapolate the scatter through four to five standard deviations to achieve exceptional levels of safety, or how to improve the property so that it is no longer a limiting feature of the design and is, therefore, irrelevant. Numbers are often important, but even more often they are not.

For these reasons materials scientists have learned to use several different kinds of "theory" to treat mechanical behavior, each of which addresses the problem at a level that is appropriate to satisfy a particular set of technological or scientific needs. I think it is possible to gather these into three categories. In order of increasing complexity, these categories include "critical flaw" models, "pattern recognition" models, and constitutive equations. The future of materials science requires the creative development of each.

"Critical flaw" models. The structure-property relations that are most widely used in the development of new materials are "critical flaw" models in which one settles on a single, critical aspect of the microstructure and works to improve it. A common way of doing this is to make the material, bend or break it, do the failure analysis to find the weak link in the microstructure, fix that, and iterate until the properties are as good as they need to be. A slight variant on this is the "some is good so more must be better" method. In this method one focuses on a microstructural feature that seems to help (such as fine grain size) and concentrates on metallurgical processing to carry it as far as one can. These ap-

proaches depend on mechanistic models, but do not ordinarily use them in an explicit way. For example, the large "supersteel" projects that are currently active in Japan and Korea have the grain refinement of steel as a central objective [19,20]. It is assumed that grain refinement will improve properties; the challenge is to accomplish it. In other words, it is accepted that, in this area, theory is well ahead of experiment.

Pattern recognition. A very large fraction of the structure-property relations that are actually used by metallurgists are essentially based on pattern recognition. If two materials have microstructures that "look alike" at some level of magnification it is expected that they will have similar mechanical behavior. If they have fracture surfaces that "look alike" it is assumed that they failed in the same way. It is for this reason that compendia such as ASM's Metals Handbook have whole volumes filled with little more than pictures of micro-structures and fracture surfaces, and engineering specifications and standards for metal parts often require more in the way of micrographs than mechanical property data.

In many cases, the pattern that is recognized is a relatively straightforward manifes-tation of a "critical flaw". For example, if a fracture surface exhibits a high population of brittle fracture features, the material ordinarily has a low fracture toughness, and fine grain size is prerequisite if a structural steel is to combine ultrahigh strength and toughness at ambient temperature.

In other cases, including many of those used in quality control, the overall pattern of the microstructure is the relevant parameter. Since, in these cases, the metallurgist often has only a qualitative sense of what he is actually doing, that is, what exactly it is about a particular microstructural pattern that is significant, it is easy to take the process as evidence of the "unscientific" nature of our field. But it is a simple fact that, in trained hands, this methodology works fairly well. Metallurgists do regularly and confidently predict mechanical properties from nothing more than an etched and magnified view of a cross-section of a material. Smart people don't denigrate techniques that work; they try to un-derstand them.

There is a developing field of "pattern recognition" that has its own methodology and mathematics. Can we use that methodology to translate a "feel" for microstructure into a set of recipes that are well grounded in mathematics and hard science? The materials community has tried over the years, without a lot of success. We've tried quantitative stereology, fractals and "expert systems", among many other methods, to get some useful handle on the patterns of microstructure. To me, the "expert system" approach seemed particularly promising, since it is based on codifying associations rather than quantitative relations. But when I became involved in a formal program to develop "expert systems" some years ago I found it frustratingly difficult to communicate with the computer scientists who were responsible for the software. I am convinced there is gold to be mined in this general area, and that it is important to find it. An approach that just might work is to de-velop simple mechanical models that incorporate microstructures than can be varied in many ways and studied from both "focused" and "defocused" perspectives to clarify how we find the patterns that matter.

Microstructure-based constitutive equations.   The highest level of the structure-property relations are constitutive equations that relate properties to a set of quantifiable variables that includes a subset that represents the microstructure. The constitutive equation may be intended for analytical use, to guide experiment or materials development, or it may be intended for use on some computational code that models the performance of an engineering system. In either case, the microstructural variables must be few and simple in form. That is, it must be possible to represent an enormously complex microstructure with only a few variables.

The development of probative constitutive equations is clearly an important objective of materials research and it is, therefore, important to consider the circumstances under which tractable constitutive equations may exist. I can identify only three situations in which it is realistic to expect that the microstructure has a simple parametric representation. The constitutive equation may apply to a series of microstructures that have a simple geometric relation to one another (in which case the microstructural parameters are geometric "scaling relations"), it may describe a mechanism that depends on the microstructure in a very simple way, or microstructure and mechanism may combine to yield an "entropic" variable that governs their relation to one another.

It would take a much longer paper than this to discuss the nature and use of constitutive equations in any moderately comprehensive way, so I will restrict this discussion to a few important and well-known examples.

The most widely used constitutive equations in metallurgy are the Hall-Petch relation

$$\sigma = \sigma_0 + Kd^{-1/2} \tag{1}$$

where d is the mean grain size (there is a similar relation for the ductile-brittle transition), and the universal hardening law

$$\sigma = \sigma_0 + \alpha Gb\sqrt{\rho} \tag{2}$$

where ρ is the average dislocation density. While their mechanistic origins are not entirely clear, both appear to be scaling relations; they are simple because they apply to self-similar microstructures.

The meaning of the Hall-Petch relation, in particular, has become an important issue in recent years as metallurgists have sought very high strength through grain refinement. The Hall-Petch relation has proven surprisingly general, even in its extensions to submicron particle sizes [21,22]. While the relation does fail at very small grain sizes, recent research suggests that this may be due to changes in the pattern of he microstructure at nanoscale grain sizes [23], as well as to changes in the mechanisms of hardening (for example, the intrusion of grain boundary sliding as a significant deformation mode [21]).

The Hall-Petch relation for the ductile-brittle transition is less well studied, despite its importance in mechanical metallurgy. The relevant work that has recently begun to appear emphasizes the nucleation of cleavage fracture [23-25], suggesting that it is the extremal grain size, rather than the mean, that is important. But if we treat the relation as a scaling law for similar microstructures, the mechanistic distinction is not important; the mean and the extrema scale together.

If these are, in fact, scaling relations it is important to know how robust they are; for example, how much can the microstructure vary before the Hall-Petch relation loses its value? The very little relevant work I have been able to find addresses only the strength, and is not entirely clear [27], though it does seem to show that significant changes in the microstructural pattern change the relation significantly. I can find no relevant modeling work on the Hall-Petch relation for the ductile-brittle transition, despite its importance in mechanical metallurgy.

A second set of constitutive equations that is widely used are the various "power-law" relations that govern steady-state creep [28]. In this case, the high homologous temperature at which creep occurs seems to blur the microstructure dependence so that simple equations are possible. But the mechanistic sources of these equations remains somewhat obscure. A large part of the data can be fit with equations that involve nothing more than Taylor expansions for the dislocation density and velocity, with the caveat that ρ be even in τ while v is odd. Other derivations assume very specific dislocation-dislocation interactions [29]. The resolution of these issues may be one of the more useful short-term applications of the multiple-dislocation models that are now being developed.

Thirdly, simple constitutive laws may result from scaling relations of the "entropic" type, in which mechanism and microstructure combine to yield a process described by a simple set of parameters. The prototypic example is E.W. Hart's classic "hardness" parameter [30], which is derived from a Caratheodory-like analysis that assumes the existence of an integrating factor for the strain. Mecking, Kocks, Follensbee and others [31,32] have built models with a similar kind of variable. Mining a different vein, Chrzan and co-workers have recently found scaling laws for deformation of intermetallic compounds [33] and multilayered films [34] by techniques like those used for the analysis of critical phenomena in phase transformations. Interestingly, in this case the scaling parameters emerge from the numerical model rather than being assumed into it, which may foreshadow how "numerical experiments" will be used in the future.

Now consider how constitutive equations are used. In many cases they are used directly, to guide materials development or "critical flaw" analyses of materials behavior. For example, the Hall-Petch relation and the various obstacle hardening laws can be used and compared to estimate the strength increment that could be obtained through various microstructural changes, and judge, for example, whether grain refinement or precipitation hardening is a more promising path to a desired improvement in a particular alloy. As we refine our understanding and appreciation for the form and limits of these constitutive equations, they will become increasingly useful for these engineering purposes.

The other use of constitutive equations is in materials modeling. It is in this area that the most dramatic progress is being made, as we use the powerful new computing machines to simulate increasingly complex materials behaviors. The simulations, again, are done with two very different objectives in mind. Quantitative models seek to predict the actual behavior of real systems. Those that use continuum models to predict the general performance of engineering systems have become very powerful and useful. However, it is at least this author's observation that they tend to become less accurate as they become more detailed, and it is difficult to find examples of accurate, quantitative models that treat microstructural effects in any detail.

But while the microstructural models may not produce accurate numbers for the behavior of real materials, they do, if properly constructed, give very accurate representations of hypothetical behavior in an ideal universe in which their constitutive equations are precisely obeyed. If one couples this accuracy with the fact that computer models can be exactly reproduced, and stopped or reversed at any point to determine precisely why some particular event occurred, it becomes evident that well-constructed simulations are powerful numerical "experiments" that can be uniquely informative in clarifying fundamental mechanisms and their interactions with one another. Viewed as an experimental tool, computer simulation has come to play important role in materials research, and will inevitably increase in importance in the future.

CONCLUSION

If we are to develop useful theories of the mechanical behavior of materials we must accept the complexity of the problem and use the full range of available tools to construct appropriate models. A few, limiting problems in the mechanical behavior of real materials can be solved exactly. They should be identified, solved and the solutions exploited to clarify a broader range of mechanical behavior. However, most of the problems that we encounter in the effort to understand, predict and improve mechanical properties are inherently unsolvable, in the strict sense of the word "solution". Still, many of them can be solved in the practical sense if we carefully analyze what is actually needed to phrase a useful solution, and employ techniques, such as critical flaw analysis, microstructural pattern recognition and probative constitutive modeling, that can provide useful answers without exact numerical solutions. This is, in fact, the way materials science has worked to achieve the substantial progress we have made. To maximize our future progress, it is important to recognize that we act in this way, not because our field is primitive or unscientific, but because it is the natural and appropriate way to drain the swamp in which we live.

ACKNOWLEDGMENTS

REFERENCES

[1]   M. L. Cohen, <u>Mat. Sci. Eng. A</u>, **105-106**, 11 (1987).

[2]   C. Krenn, J.W. Morris, Jr., S.-H. Jhi, and J. Ihm, in *Hard Coatings Based on Borides, Carbides & Nitrides*, Kumar, Chung and Chia, eds., TMS, 1998, p. 379.

[3]   F.R.N. Nabarro, <u>Phil. Mag.A</u>, **75**, 703 (1997)

[4]   U.F. Kocks, A.S. Argon and M.F. Ashby, <u>Thermodynamics and Kinetics of Slip</u>, Pergamon, Oxford (1975) (Vol. 19 in <u>Progress in Materials Science</u>, Chalmers, Christian and Massalski, eds.)

[5]   A. Kelly and N.H. Macmillan, <u>Strong Solids</u>, Clarendon Press, Oxford (1986)

[6]   T. Paxton, P. Gumbsch, and M. Methfessel, <u>Phil. Mag. Lett.</u>, **63**, 267 (1991)

[7]   D. Roundy, C.R. Krenn, M.L. Cohen and J.W. Morris, Jr., <u>Phys. Rev. Lett</u>., **82**, 2713-16 (1999)

[8]   S.-H. Jhi, J. Ihm, S.-G. Louie and M.L. Cohen, <u>Nature</u>, <u>399</u>, 132 (1999)

[9]   R. Hill and F. Milstein, <u>Phys. Rev. B</u>, <u>15</u>, 3087-97 (1977)

[10]   W. Xu and J.A. Moriarty, <u>Phys. Rev. B</u>, **54**, 6941 (1996)

[11]   Y. Sun and E. Kaxiras, <u>Phil. Mag. A</u>, **75**, 1117 (1997)

[12]   M. Sob, L.G. Wang and V. Vitek , <u>Mat. Sci. Eng. A</u>, **234-236**, 1075 (1997)

[13]   W. Li and T. Wang, <u>J. Phys.: Condensed Matter</u>, **10**, 9889-9904 (1998)

[14]   D. Roundy and M.L. Cohen, University of California, Berkeley, unpublished research (1999)

[15]   C.R. Krenn, D. Roundy, J.W. Morris, Jr. and M.L. Cohen, "The non-linear elastic behavior and ideal shear strength of Al and Cu", <u>Mat. Sci. Eng. A</u>, (in press)

[16]   V.V. Bulatov, S. Yip and A.S. Argon, <u>Phil. Mag. A</u>, **72**, 453 (1995)

[17]   D.C. Chrzan and K. Lin, University of California, Berkeley, unpublished research (1999)

[18]   J.E. Shigley and C.R. Mischke, <u>Mechanical Engineering Design</u>, Fifth Edition, McGraw-Hill, New York, 1989

[19]   "Frontier Research Center for Structural Materials", National Research Institute for Metals, Tsukuba, Japan 1997

[20]   W.-Y. Choo, POSCO, Pohang, Korea, Private Communication (1999)

[21]   Y. Kimura and S. Takaki, in <u>Proceedings, 1998 PM World Congress: Nanocrystalline Materials</u>, p. 573

[22]   J.S.C. Jang and C.C. Koch, <u>Scr. Metall. Mater.</u>, **24**, 1599 (1990)

[23]   J.R. Weertman, P.G. Sanders and C.J. Youngdahl, <u>Mat. Sci. Eng. A</u>, **234-6** , 77, 1997

[24]   G.Z. Wang, J.H. Chen and Z.H. Li, <u>Met. Trans.</u>, **28A**, 1689 (1997)

[25]   T. Tani and M. Naguno, <u>Met. Trans.</u>, **26A**, 391 (1994)

[26]   J.W. Morris, Jr., <u>Mat. Res. Soc. Proc.</u>, **539**, 23-27 (1999)

[27]   K.J. Kurzydlowski and J.J. Bucki, <u>Acta Met.</u>, **41**, 3141 (1993)

[28]   J.E. Bird, A.K. Mukherjee and J.E. Dorn, in <u>Quantitative Relation between Properties and Microstructure</u>, Isreal Universities Press, Haifa, Israel (1969) p. 255

[29]   J. Weertman, <u>Trans. ASM</u>, **61**, 681 (1968)

[30]   E.W. Hart, <u>Acta Met</u>, **18**, 599 (1970)

[31]   H. Mecking and U.F. Kocks, <u>Acta Met.</u>, **29**, 1865 (1981)

[32]   P.S. Follensbee and U.F. Kocks, <u>Acta Met.</u>, **36**, 81 (1988)

[32]   D.C. Chrzan and M.S. Daw, <u>Phys. Rev. B</u>, **55**, 798 (1997)

[33]   L.H. Friedman and D.C. Chrzan, <u>Phys. Rev. Lett.</u>, **81**, 2715 (1998)